# Next-to-leading ultrasoft running of the heavy quarkonium potentials and spectrum: Spin-independent case

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# Abstract

We compute the next-to-leading logarithmic (NLL) ultrasoft running of the spin-independent singlet potentials up to  $\mathcal{O}(1/m^2)$ , and the corresponding contribution to the spectrum. This includes the static energy at next-to-next-to-leading logarithmic (NNNLL) order. As a byproduct of these results we set the stage for the complete analytic and numerical computation of the heavy quarkonium spectrum with N<sup>3</sup>LL accuracy for  $l \neq 0$  (angular momentum) and s = 0 (spin) states. We also compute the next-to-next-to-next-to-next-to-leading order (N<sup>4</sup>LO) ultrasoft spin-independent contribution to the heavy quarkonium mass and static energy.

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#### I. INTRODUCTION

The evaluation of the three-loop soft contribution to the static potential [1, 2] has given the final piece needed for the complete evaluation of the heavy quarkonium spectrum at NNNLO [3, 4]. This result is also necessary for the long term project of obtaining the heavy quarkonium spectrum with NNNLL accuracy<sup>1</sup>, and the non-relativistic sum rules and t- $\bar{t}$  production near threshold with NNLL/NNNLO one. It is then timely to compute the next-to-leading ultrasoft running of the potentials, as it enters in the evaluation of the previously mentioned observables with such precision. Therefore, in this paper we compute the next-to-leading ultrasoft running of the spin-independent potentials. For the static potential the running has already been computed in Ref. [7], we confirm this result, for the 1/m and  $1/m^2$  potentials the result is new.

We will write the results for the potentials in position space. This could be eventually convenient for future numerical evaluations of decays and sum rules. Moreover, such computation is interesting on its own, as it shows the subtleties appearing in the explicit matching (and the associated scheme dependence) between the soft and ultrasoft computation. In momentum space this discussion has already been made in Ref. [3], we do so in position space (see also Ref. [8] for a similar discussion for the QCD static potential in three dimensions, and Ref. [9] for the SUSY QCD static potential). This discussion is relevant, as the subtraction scheme of the ultrasoft divergences could be different in position and momentum space.

The basis of potentials that we use for the 1/m and  $1/m^2$  potentials is redundant. Therefore, the expression obtained for each potential is ambiguous, since field redefinitions can shift some contributions from the 1/m to the  $1/m^2$  potentials, and viceversa. In principle, one could avoid this problem by considering all the 1/m and  $1/m^2$  potentials as a whole. Yet, this observation has implications in one of the possible applications of our result: comparison (at short distances) with the recent lattice simulations of the 1/m and  $1/m^2$  potentials obtained in Refs. [10, 11] using their non-perturbative expression in terms of Wilson loops [12, 13]. Unfortunately, the ambiguity just mentioned makes not possible a direct connection between the non-perturbative expressions of the potentials in terms of Wilson loops and the

<sup>&</sup>lt;sup>1</sup> Actually, this accuracy has already been achieved for the hyperfine splitting [5, 6].

perturbative computation. This would require a dedicated study that goes beyond the aim of this work.

Whereas there are still some pieces left for a complete NNNLL evaluation of the heavy quarkonium spectrum, our result provides the missing link for the complete result for  $l \neq 0$  and s = 0 states, the structure of which is given in this paper for the first time. The full explicit analytic form will be presented elsewhere. Another by-product of our computation is the N<sup>4</sup>LO ultrasoft spin-independent contribution to the heavy quarkonium mass.

The next-to-leading ultrasoft running of the  $1/m^2$  potential was computed in Ref. [14] in a different framework named vNRQCD (see Refs. [15–17]). The computation of such object alone does not make much sense due to field redefinitions ambiguities that can shift contributions among different potentials. If we compare expressions for the  $1/m^2$  potential, we disagree with the running of  $V_{\bf p^2}^{(2)}$  obtained in that paper but yet, as mentioned, this could be due to field redefinition ambiguities. In Ref. [18] the  $1/m^2$  and 1/m potentials were considered. Nevertheless, no definite outcome for the complete NLL ultrasoft running of the potentials was obtained. The reason was that the result was dependent on how the infrared divergences were regulated, so they even ended up having more than one possible result. Thus, a complete comparison with their results at this stage is not possible. Other issues that complicate the comparison are that the soft contribution is not included in their potential and the intrinsic scheme dependence. Either way, we believe that such future comparison should be better performed for specific observables. In this respect a future evaluation of the heavy quarkonium spectrum with NNNLL accuracy for  $l \neq 0$  and s = 0 states with vNRQCD would be a good object for such comparison.

Non-perturbative effects will not be considered in this paper and ultrasoft effects will be computed within perturbation theory (i.e. in the  $m\alpha^2 \gg \Lambda_{\rm QCD}$  limit), yet the renormalization group (RG) results will also be valid when  $m\alpha^2 \sim \Lambda_{\rm QCD}$ . The ultrasoft effects can be easily obtained in the non-equal mass case, as they only depend on the reduced mass. On the other hand the full soft contribution is only known in the equal mass case at the appropriate order.

The outline of the paper is as follows. In Sec. II we introduce the theoretical setup and show some bare results relevant for our computation. In Sec. III we compute the ultrasoft correction to the spin-independent Hamiltonian with NLL precision and give explicit expres-

sions for the relevant potentials. In Sec. IV we give expressions for the heavy quarkonium energy and static potential with NNNLL precision (for the heavy quarkonium mass only when  $l \neq 0$  and s = 0), and in Sec. V we present our conclusions. Finally, in the Appendix we gather some constants that appear throughout the computation.

#### II. PNRQCD

Up to NLO in the multipole expansion the effective Lagrangian density of pNRQCD takes the form [19, 20]:

$$\mathcal{L}_{us} = \text{Tr}\left\{S^{\dagger} \left(i\partial_{0} - h_{s}(r)\right)S + O^{\dagger} \left(iD_{0} - h_{o}(r)\right)O\right\}$$

$$+gV_{A}(r)\text{Tr}\left\{O^{\dagger}\mathbf{r} \cdot \mathbf{E}S + S^{\dagger}\mathbf{r} \cdot \mathbf{E}O\right\} + g\frac{V_{B}(r)}{2}\text{Tr}\left\{O^{\dagger}\left\{\mathbf{r} \cdot \mathbf{E}, O\right\}\right\}.$$

$$(1)$$

We define color singlet and octet fields for the quark-antiquark system by  $S = S(\mathbf{r}, \mathbf{R}, t)$  and  $O^a = O^a(\mathbf{r}, \mathbf{R}, t)$ , respectively.  $\mathbf{R} \equiv \frac{m_1}{m_1 + m_2} \mathbf{x}_1 + \frac{m_2}{m_1 + m_2} \mathbf{x}_2$  is the center position of the system, and  $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$ . In order for S and  $O^a$  to have the proper free-field normalization in color space they are related to the fields in Eq. (1) as follows:

$$S \equiv \frac{\mathbf{1}_c}{\sqrt{N_c}} S$$
,  $O \equiv \frac{T^a}{\sqrt{T_F}} O^a$ . (2)

All gluon and scalar fields in Eq. (1) are evaluated in **R** and the time t, in particular the chromoelectric field  $\mathbf{E} \equiv \mathbf{E}(\mathbf{R}, t)$  and the ultrasoft covariant derivative  $iD_0O \equiv i\partial_0O - g[A_0(\mathbf{R}, t), O]$ .

 $h_s$  can be split in the kinetic term and the potential:

$$h_s(\mathbf{r}, \mathbf{p}, \mathbf{S}_1, \mathbf{S}_2) = \frac{\mathbf{p}^2}{2 m_r} + V_s(\mathbf{r}, \mathbf{p}, \mathbf{S}_1, \mathbf{S}_2), \tag{3}$$

$$h_o(\mathbf{r}, \mathbf{p}, \mathbf{S}_1, \mathbf{S}_2) = \frac{\mathbf{p}^2}{2 m_r} + V_o(\mathbf{r}, \mathbf{p}, \mathbf{S}_1, \mathbf{S}_2), \tag{4}$$

where  $m_r = m_1 m_2/(m_1 + m_2)$ ,  $\mathbf{p} = -i \nabla_{\mathbf{r}}$  and  $\mathbf{S}_1$  and  $\mathbf{S}_2$  are the spin of the quark and the antiquark respectively. For the equal mass case:  $m_1 = m_2 = m$ , the potential has the following structure (we drop the labels s and o for the singlet and octet, which have to be understood):

$$V(r) = V^{(0)}(r) + \frac{V^{(1)}(r)}{m} + \frac{V^{(2)}}{m^2} + \cdots,$$
 (5)

$$V^{(2)} = V_{SD}^{(2)} + V_{SI}^{(2)},$$

$$V_{SI}^{(2)} = \frac{1}{2} \left\{ \mathbf{p}^{2}, V_{\mathbf{p}^{2}}^{(2)}(r) \right\} + \frac{V_{\mathbf{L}^{2}}^{(2)}(r)}{r^{3}} \mathbf{L}^{2} + V_{r}^{(2)}(r),$$

$$V_{SD}^{(2)} = V_{LS}^{(2)}(r) \mathbf{L} \cdot \mathbf{S} + V_{S^{2}}^{(2)}(r) \mathbf{S}^{2} + V_{\mathbf{S}_{12}}^{(2)}(r) \mathbf{S}_{12}(\hat{\mathbf{r}}),$$
(6)

where  $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ ,  $\mathbf{S}_{12}(\hat{\mathbf{r}}) \equiv 4(3\hat{\mathbf{r}} \cdot \mathbf{S}_1 \hat{\mathbf{r}} \cdot \mathbf{S}_2 - \mathbf{S}_1 \cdot \mathbf{S}_2)$ , and  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ . The last two equalities hold in 4 dimensions.  $\mathbf{L}^2$  is generalized to  $(\mathbf{q} = \mathbf{p} - \mathbf{p}')$ 

$$\frac{\mathbf{L}^2}{2\pi r^3} \to \left(\frac{\mathbf{p}^2 - \mathbf{p}'^2}{\mathbf{q}^2}\right)^2 - 1 \tag{8}$$

to be compatible with D dimensional calculations in momentum space. In this paper we focus on the ultrasoft corrections to the spin-independent singlet potentials. Therefore, we will not consider Eq. (7) (nor its generalization to D dimensions, see for instance Ref. [21]) in the following and drop the labels s and o, except for the static potentials.

From now on we will use the index "B" to explicitly denote bare quantities. Parameters without this index are understood to be renormalized. The bare parameters of the theory are  $\alpha_B$  ( $g_B$ ) and the potentials, generically denoted by  $V_B$ .  $\alpha$  and  $V_{\{s,o,A,B\}}(r)$  are the Wilson coefficients of the effective Lagrangian. They are fixed at a scale  $\nu$  smaller than (or similar to) 1/r and larger than the ultrasoft and any other scale in the problem by matching pNRQCD and NRQCD.

In our convention  $\alpha_B$  is dimensionless and related to  $g_B$  by  $(D = d + 1 = 4 + 2\epsilon)$ 

$$\alpha_B = \frac{g_B^2 \nu^{2\epsilon}}{4\pi} \,, \tag{9}$$

where  $\nu$  is the renormalization scale. It has a special status since it does not receive corrections from other Wilson coefficients of the effective theory. We renormalize it multiplicatively:

$$\alpha_B = Z_\alpha \alpha \,, \tag{10}$$

where

$$Z_{\alpha} = 1 + \sum_{s=1}^{\infty} Z_{\alpha}^{(s)} \frac{1}{\epsilon^s} \,. \tag{11}$$

The RG equation of  $\alpha$  is

$$\nu \frac{d}{d\nu} \alpha \equiv \alpha \beta(\alpha; \epsilon) = 2\epsilon \alpha + \alpha \beta(\alpha; 0). \tag{12}$$

In the limit  $\epsilon \to 0$ 

$$\nu \frac{d}{d\nu} \alpha \equiv \alpha \beta(\alpha; 0) \equiv \alpha \beta(\alpha) = -2\alpha \frac{d}{d\alpha} Z_{\alpha}^{(1)}, \qquad (13)$$

where

$$Z_{\alpha}^{(1)} = \frac{\alpha}{4\pi} \beta_0 + \cdots \qquad \alpha \beta(\alpha) = -2\alpha \left( \beta_0 \frac{\alpha}{4\pi} + \beta_1 \frac{\alpha^2}{(4\pi)^2} + \cdots \right) , \qquad (14)$$

and expressions for  $\beta_0$ ,  $\beta_1$ , etc, can be found in the Appendix.

The bare potentials  $V_B$  in position space have integer mass dimensions (note that this is not so in momentum space) and, due to the structure of the theory, we do not renormalize them multiplicatively (see the discussion in Ref. [22]). We define

$$V_B = V + \delta V. (15)$$

 $\delta V$  will generally depend on the (matching) coefficients of the effective theory, i.e. on  $\alpha$  and V, and on the number of space-time dimensions. In D dimensions, using the MS renormalization scheme, we define

$$\delta V = \sum_{s=1}^{\infty} Z_V^{(s)} \frac{1}{\epsilon^s} \,. \tag{16}$$

From the scale independence of the bare potentials

$$\nu \frac{d}{d\nu} V_B = 0, \qquad (17)$$

one obtains the RG equations of the different renormalized potentials. They can schematically be written as one (vector-like) equation including all potentials:

$$\nu \frac{d}{d\nu} V = B(V) \,, \tag{18}$$

$$B(V) \equiv -\left(\nu \frac{d}{d\nu} \delta V\right) \,. \tag{19}$$

Note that Eq. (18) implies that all the  $1/\epsilon$  poles disappear once the derivative with respect to the renormalization scale is performed. This imposes some constraints on  $\delta V$ :

$$\mathcal{O}(1/\epsilon): \qquad B(V) = -2\alpha \frac{\partial}{\partial \alpha} Z_V^{(1)}, \qquad (20)$$

$$\mathcal{O}(1/\epsilon^2): \qquad B(V)\frac{\partial}{\partial V}Z_V^{(1)} + \alpha\beta(\alpha)\frac{\partial}{\partial \alpha}Z_V^{(1)} + 2\alpha\frac{\partial}{\partial \alpha}Z_V^{(2)} = 0, \qquad (21)$$

and so on.

Out of this theory we can obtain some observables. In this paper we focus on the energy of the heavy quarkonium (also in its static limit). The singlet propagator near on-shell can be approximated to the following expression

$$\int dt e^{iEt} d^3R \langle vac|S(t, \mathbf{r}, \mathbf{R})S^{\dagger}(0, \mathbf{r}', \mathbf{0})|vac\rangle \sim \phi_n(\mathbf{r})\phi_n(\mathbf{r}')\langle n|\frac{i}{E - h_s^B - \Sigma_B(E) + i\epsilon}|n\rangle$$

$$\sim \phi_n(\mathbf{r})\phi_n(\mathbf{r}')\frac{i}{E - E_n^{pot} - \delta E_n^{us} + i\epsilon}, \qquad (22)$$

where n generically denotes the quantum number of the bound state:  $n \to (n \text{ (principal quantum number)}, l \text{ (orbital angular momentum)}, s \text{ (total spin)}, j \text{ (total angular momentum)}$ ).  $E_n^{pot}$  and  $\phi_n(\mathbf{r})$  are the eigenvalue and eigenfunction respectively of the equation

$$h_s \phi_n(\mathbf{r}) = E_n^{pot} \phi_n(\mathbf{r}) \tag{23}$$

and, in general, will depend on the renormalization scheme the ultrasoft computation has been performed with. The self-energy  $\Sigma_B(E)$  accounts for the effects due to the ultrasoft scale and can be expressed in a compact form at NLO in the multipole expansion (but exact to any order in  $\alpha$ ) through the chromoelectric correlator. It reads (in the Euclidean)

$$\Sigma_B(E) = V_A^2 \frac{T_F}{(D-1)N_c} \int_0^\infty dt \mathbf{r} e^{-t(h_o^B - E)} \mathbf{r} \langle vac| g \mathbf{E}_E^a(t) \phi_{\text{adj}}^{ab}(t, 0) g \mathbf{E}_E^b(0) | vac \rangle. \tag{24}$$

The pNRQCD one-loop computation yields [23–25]

$$\Sigma_B(1 - \text{loop}) = -g^2 C_f V_A^2(1 + \epsilon) \frac{\Gamma(2 + \epsilon)\Gamma(-3 - 2\epsilon)}{\pi^{2 + \epsilon}} \mathbf{r} \left(h_o^B - E\right)^{3 + 2\epsilon} \mathbf{r}.$$
 (25)

The two-loop bare expression can be trivially deduced from the results obtained in Refs. [26–28] for the static case. It reads

$$\Sigma_B(2 - \text{loop}) = g^4 C_f C_A V_A^2 \Gamma(-3 - 4\epsilon) \left[ \mathcal{D}^{(1)}(\epsilon) - (1 + 2\epsilon) \mathcal{D}_1^{(1)}(\epsilon) \right] \mathbf{r} \left( h_o^B - E \right)^{3+4\epsilon} \mathbf{r} , \quad (26)$$

where

$$\mathcal{D}^{(1)}(\epsilon) = \frac{1}{(2\pi)^2} \frac{1}{4\pi^{2+2\epsilon}} \Gamma^2(1+\epsilon) g(\epsilon) , \qquad (27)$$

$$\mathcal{D}_{1}^{(1)}(\epsilon) = \frac{1}{(2\pi)^{2}} \frac{1}{4\pi^{2+2\epsilon}} \Gamma^{2}(1+\epsilon) g_{1}(\epsilon) , \qquad (28)$$

and

$$g(\epsilon) = \frac{2\epsilon^3 + 6\epsilon^2 + 8\epsilon + 3}{\epsilon (2\epsilon^2 + 5\epsilon + 3)} - \frac{2\epsilon\Gamma(-2\epsilon - 2)\Gamma(-2\epsilon - 1)}{(2\epsilon + 3)\Gamma(-4\epsilon - 3)},$$
(29)

$$g_1(\epsilon) = \frac{6\epsilon^3 + 17\epsilon^2 + 18\epsilon + 6}{\epsilon^2 (2\epsilon^2 + 5\epsilon + 3)} + \frac{4(\epsilon + 1)n_f T_F}{\epsilon (2\epsilon + 3)N_c} + \frac{2(\epsilon^2 + \epsilon + 1)\Gamma(-2\epsilon - 2)\Gamma(-2\epsilon - 1)}{\epsilon (2\epsilon + 3)\Gamma(-4\epsilon - 3)}. \quad (30)$$

From  $\Sigma_B(E)$  it is possible to obtain  $\delta E_n^{us}$ . This will be discussed in the following sections.

In principle we should also consider possible soft and ultrasoft corrections to  $V_A$ . Those have been studied in Ref. [22] with LL accuracy, in Ref. [27] with NLO accuracy, and in Ref. [7] with NLL accuracy, reaching to the conclusion that they do not contribute to the precision of our computation (so we can set  $V_A = 1$ ):

$$\nu \frac{d}{d\nu} V_A = 0 + \mathcal{O}(\alpha^3) \,, \tag{31}$$

whereas for the initial matching condition  $V_A = 1 + \mathcal{O}(\alpha^2)$ .

## III. $V_s$

#### A. Ultrasoft running

We now discuss how to obtain the ultrasoft RG running of  $V_s$  from  $\Sigma_B(E)$ . The bare ultrasoft self-energy is a function of  $h_o - E$ ,  $\alpha$  and  $\epsilon$ , where this  $\alpha$  refers to the one associated to the ultrasoft running. The  $\alpha$  associated to the soft running is encoded in the matching coefficients (i.e. the potentials). From the combined one and two loop ultrasoft computation we obtain (after changing the bare alpha by the renormalized one)

$$\Sigma_{B}(E) = -\frac{1}{\epsilon^{2}} C_{f} V_{A}^{2} \mathbf{r} (h_{o} - E)^{3} \mathbf{r} \frac{2}{3} \beta_{0} \frac{\alpha^{2}(\nu)}{(4\pi)^{2}}$$

$$-\frac{1}{\epsilon} C_{f} V_{A}^{2} \mathbf{r} (h_{o} - E)^{3} \mathbf{r} \left[ \frac{\alpha(\nu)}{3\pi} - \frac{\alpha^{2}(\nu)}{36\pi^{2}} (C_{A} (-\frac{47}{3} - 2\pi^{2}) + \frac{10}{3} T_{F} n_{f}) \right]$$

$$+ C_{f} V_{A}^{2} \mathbf{r} (h_{o} - E)^{3} \left[ -\frac{\alpha(\nu)}{9\pi} \left( 6 \ln \left( \frac{h_{o} - E}{\nu} \right) + 6 \ln 2 - 5 \right) \right]$$

$$+ \frac{\alpha^{2}(\nu)}{108\pi^{2}} \left( 18\beta_{0} \ln^{2} \left( \frac{h_{o} - E}{\nu} \right) - 6 \left( C_{A} \left( 13 + 4\pi^{2} \right) + 2\beta_{0} (5 - 3 \ln 2) \right) \ln \left( \frac{h_{o} - E}{\nu} \right) \right)$$

$$-2C_{A} \left( -84 + 39 \ln 2 + 4\pi^{2} (-2 + 3 \ln 2) + 72\zeta(3) \right)$$

$$+ \beta_{0} \left( 67 + 3\pi^{2} - 60 \ln 2 + 18 \ln 2 \right) \right] \mathbf{r} + \mathcal{O}(\epsilon, \alpha^{3}).$$
(32)

Note that the  $1/\epsilon^2$  term comes from two sources: the two loop bare result and the  $1/\epsilon$  inside  $\alpha_B$  in the one loop ultrasoft. Quite remarkably, there is no log dependence of the  $1/\epsilon$  and  $1/\epsilon^2$  terms. This is of fundamental importance for renormalizability and a check of

consistency. This result has to be reexpressed in terms of the potentials of the singlet/octet Hamiltonian and  $h_s - E$ . Positive powers of  $h_s - E$  do not contribute to the energy, as they cancel powers of  $1/(h_s - E)$  in the Green function. Therefore, we are rather interested in the identity (valid in D dimensions)

$$\mathbf{r}(h_o - E)^3 \mathbf{r} = \mathbf{r}^2 (\Delta V)^3 - \frac{1}{2m_r^2} \left[ \mathbf{p}, \left[ \mathbf{p}, V_o^{(0)} \right] \right] + \frac{1}{2m_r^2} \left\{ \mathbf{p}^2, \Delta V \right\} + \frac{2}{m_r} \Delta V \left( r \frac{d}{dr} V_s^{(0)} \right)$$

$$+ \frac{1}{2m_r} \left[ (\Delta V)^2 (3d - 5) + 4\Delta V \left( \left( r \frac{d}{dr} \Delta V \right) + \Delta V \right) + \left( \left( r \frac{d}{dr} \Delta V \right) + \Delta V \right)^2 \right]$$

$$+ \mathcal{O}((h_s - E)),$$
(33)

where we have approximated  $h_o - h_s = V_o^{(0)} - V_s^{(0)}$ , which is enough for our precision, and defined  $\Delta V \equiv V_o^{(0)} - V_s^{(0)}$ . We have used the combination  $\left(\left(r\frac{d}{dr}\Delta V\right) + \Delta V\right)$ , since it has a  $\mathcal{O}(\epsilon)$  suppression with respect to  $\Delta V$ . Note that in D dimensions the static potential has the following expansion in terms of the bare coupling constant  $(C_s \equiv -C_F \text{ and } C_o \equiv 1/(2N_c))$ :

$$V_{s/o,B}^{(0)} = C_{s/o} g_B^2 \sum_{n=0}^{\infty} \frac{g_B^{2n} c_n^{(s/o)}(D) r^{-2(n+1)\epsilon}}{r} . \tag{34}$$

We can now obtain the counterterms of the singlet Hamiltonian due to the ultrasoft divergences up to NLO in the following compact expression

$$\delta V_{s} = \left(\mathbf{r}^{2}(\Delta V)^{3} - \frac{1}{2m_{r}^{2}}\left[\mathbf{p},\left[\mathbf{p},V_{o}^{(0)}\right]\right] + \frac{1}{2m_{r}^{2}}\left\{\mathbf{p}^{2},\Delta V\right\} + \frac{2}{m_{r}}\Delta V\left(r\frac{d}{dr}V_{s}^{(0)}\right) \right. \\
\left. + \frac{1}{2m_{r}}\left[(\Delta V)^{2}(3d-5) + 4\Delta V\left(\left(r\frac{d}{dr}\Delta V\right) + \Delta V\right) + \left(\left(r\frac{d}{dr}\Delta V\right) + \Delta V\right)^{2}\right]\right) \\
\times \left[\frac{1}{\epsilon}C_{f}V_{A}^{2}\left[\frac{\alpha(\nu)}{3\pi} - \frac{\alpha^{2}(\nu)}{36\pi^{2}}(C_{A}(-\frac{47}{3} - 2\pi^{2}) + \frac{10}{3}T_{F}n_{f})\right] + \frac{1}{\epsilon^{2}}C_{f}V_{A}^{2}\frac{2}{3}\beta_{0}\frac{\alpha^{2}(\nu)}{(4\pi)^{2}}\right]. (35)$$

The whole  $1/\epsilon^2$  term fulfills Eq. (21) and hence it is a check of the two-loop computation. In the above expressions we choose to keep the full d-dependence (also in the potentials, see Eq. (34)). This is not particularly relevant for the computations we perform in this paper, but will be potentially important once potential divergences are included, necessary for a complete NNNLL evaluation of the heavy quarkonium mass. As we have already mentioned, in this prescription we also take  $V_s^{(0)}$  and  $V_o^{(0)}$  in d dimensions. Since we only need them at one loop, the ultrasoft divergences of  $V_{s/o}^{(0)}$  do not show up yet. This actually means that the renormalized potentials are equal to their bare expressions (which one can find in Ref. [29]):

 $V_{s/o}^{(0)} \simeq V_{s/o,B}^{(0)}$ , and  $V_{s/o,B}^{(0)}$  are finite when we take the  $\epsilon \to 0$  limit. Moreover, at one loop, we also have the equality  $V_o^{(0)} = -1/(N_c^2 - 1)V_s^{(0)}$ . We prefer the scheme defined by Eq. (35), since it allows to keep the ultrasoft counterterms in a very compact manner. One is always free to change to a more standard  $\overline{\rm MS}$  scheme. Note that the  $\overline{\rm MS}$  scheme in momentum and position space are different.

Using Eq. (35) and Eq. (20) we obtain the following RG equation that resums the ultrasoft logs of the potential:

$$\nu \frac{d}{d\nu} V_{s,\overline{\rm MS}} = B_{V_s} \,, \tag{36}$$

where

$$B_{V_s} = C_f V_A^2 \left[ \mathbf{r}^2 (\Delta V)^3 + \frac{2}{m_r} \left( \Delta V \left( r \frac{d}{dr} V_s^{(0)} \right) + (\Delta V)^2 \right) - \frac{1}{2m_r^2} \left[ \mathbf{p}, \left[ \mathbf{p}, V_o^{(0)} \right] \right] \right]$$

$$+ \frac{1}{2m_r^2} \left\{ \mathbf{p}^2, \Delta V \right\} \right] \times \left[ -\frac{2\alpha(\nu)}{3\pi} + \frac{\alpha^2(\nu)}{9\pi^2} (C_A(-\frac{47}{3} - 2\pi^2) + \frac{10}{3} T_F n_f) + \mathcal{O}(\alpha^3) \right],$$
(37)

and now one could take the four-dimensional expression for the potentials. This result holds true in both schemes, the MS and  $\overline{\rm MS}$  (in a way this is due to the fact that the subdivergencies associated to  $\alpha$  also change to make the result scheme independent). After solving the RG equation we find

$$\delta V_{s,RG}(r;\nu_s,\nu) = \left[ \left( \mathbf{r}^2 (\Delta V)^3 + \frac{2}{m_r} \left( \Delta V \left( r \frac{d}{dr} V_s^{(0)} \right) + (\Delta V)^2 \right) \right) F(\nu_s;\nu) - \frac{1}{2m_r^2} \left[ \mathbf{p}, \left[ \mathbf{p}, V_o^{(0)}(r) F(\nu_s;\nu) \right] \right] + \frac{1}{2m_r^2} \left\{ \mathbf{p}^2, \Delta V(r) F(\nu_s;\nu) \right\} \right], \quad (38)$$

where we define

$$F(\nu_{s};\nu) = C_{f}V_{A}^{2}\frac{2\pi}{\beta_{0}} \left\{ \frac{2}{3\pi} \ln \frac{\alpha(\nu)}{\alpha(\nu_{s})} - (\alpha(\nu) - \alpha(\nu_{s})) \left( \frac{8}{3}\frac{\beta_{1}}{\beta_{0}} \frac{1}{(4\pi)^{2}} - \frac{1}{27\pi^{2}} \left( C_{A} \left( 47 + 6\pi^{2} \right) - 10T_{F}n_{f} \right) \right) \right\}$$

$$\simeq -C_{F}V_{A}^{2}\frac{2}{3}\frac{\alpha}{\pi} \ln \frac{\nu}{\nu_{s}} + \mathcal{O}(\alpha^{2}).$$
(39)

Note that, formally, we can set  $\nu_s = 1/r$  as far as  $F(1/r, \nu)$  is kept inside the (anti)commutators, i.e. in the way displayed in Eq. (38). Yet one should be careful, as objects that are ill defined (not even distributions) could appear. We discuss this issue further below.

From Eq. (38) we can easily identify the RG contribution to each potential<sup>2</sup> (now we work in the equal mass case). For the static potential we have

$$\delta V_{s,RG}^{(0)}(r;\nu_s,\nu) = \mathbf{r}^2 (\Delta V)^3 F(\nu_s;\nu) , \qquad (40)$$

which agrees with Ref. [7].

For the 1/m potential the RG contribution reads

$$\delta V_{s,RG}^{(1)}(r;\nu_s,\nu) = 4\left(\Delta V \left(r \frac{d}{dr} V_s^{(0)}\right) + (\Delta V)^2\right) F(\nu_s;\nu). \tag{41}$$

For the momentum-dependent  $1/m^2$  potential we have

$$\delta V_{p^2,RG}^{(2)}(r;\nu_s,\nu) = 4\Delta V(r)F(\nu_s;\nu). \tag{42}$$

The RG correction to  $V_r$  deserves a special discussion. From Eq. (38) we have

$$\delta V_{r,RG}^{(2)}(r;\nu_s,\nu) = -2\left[\mathbf{p}, \left[\mathbf{p}, V_o^{(0)} F(\nu_s;\nu)\right]\right] = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \delta \tilde{V}_{r,RG}^{(2)}(q;\nu_s,\nu),$$
(43)

where

$$\delta \tilde{V}_{r,RG}^{(2)}(q;\nu_s,\nu) = -2\mathbf{q}^2 \tilde{V}_o^{(0)}(q) F(\nu_s;\nu), \qquad (44)$$

and  $\tilde{V}_o^{(0)}$  is the Fourier transform of  $V_o^{(0)}$ . Note that we have chosen to write  $\delta V_r$  in momentum space as well. This we could also do for the previous potentials but now will be particularly convenient. The reason is that for  $\delta V_{r,RG}(r;\nu_s,\nu)$  we cannot naively set  $\nu_s=1/r$  (as we did for the previous potentials and was convenient to resum logs of r) because divergent distributions like  $\delta^{(3)}(\mathbf{r}) \ln r$  could appear. On the other hand we would like to make something analogous, as it allows to resum (and keep in a compact way) some subleading logs. We then choose to set  $\nu_s=q$  in the Fourier transform and define

$$\delta V_{r,RG}^{(2)}(r;\nu) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \delta \tilde{V}_{r,RG}^{(2)}(q;q,\nu) , \qquad (45)$$

where  $\delta \tilde{V}_{r,RG}^{(2)}(q;q,\nu)$  is Taylor expanded in powers of  $\ln q$ . We will elaborate on this expression in the following subsection (in practice we will only need the single log of this expansion). Finally also note that  $\delta V_{r,RG}^{(2)}$  vanishes in the large  $N_c$  limit.

<sup>&</sup>lt;sup>2</sup> And from previous equations one could also easily obtain the counterterms and RG equations for each potential.

## B. Initial matching conditions

The only thing left to obtain is the initial matching condition for the potential. We will only consider the spin-independent terms and stick to the equal mass case, since the matching coefficients at one loop are not known in the non-equal mass case, although many partial results exist.

We now study each potential separately. Note that the result will depend on the basis of potentials used and on field redefinitions except for the singlet static potential, which is unambiguous<sup>3</sup>.

The initial matching conditions for the static potential in our  $\overline{\rm MS}$  scheme reads

$$V_{s,\overline{\text{MS}}}^{(0)}(r;\nu) = -\frac{C_f \alpha_s(\nu)}{r} \left\{ 1 + \sum_{n=1}^3 \left( \frac{\alpha_s(\nu)}{4\pi} \right)^n a_n(\nu;r) \right\}, \tag{46}$$

with coefficients

$$a_{1}(\nu,r) = a_{1} + 2\beta_{0} \ln(\nu e^{\gamma_{E}}r) ,$$

$$a_{2}(\nu,r) = a_{2} + \frac{\pi^{2}}{3}\beta_{0}^{2} + (4a_{1}\beta_{0} + 2\beta_{1}) \ln(\nu e^{\gamma_{E}}r) + 4\beta_{0}^{2} \ln^{2}(\nu e^{\gamma_{E}}r) ,$$

$$a_{3}(\nu,r) = a_{3} + a_{1}\beta_{0}^{2}\pi^{2} + \frac{5\pi^{2}}{6}\beta_{0}\beta_{1} + 16\zeta_{3}\beta_{0}^{3}$$

$$+ \left(2\pi^{2}\beta_{0}^{3} + 6a_{2}\beta_{0} + 4a_{1}\beta_{1} + 2\beta_{2} + \frac{16}{3}C_{A}^{3}\pi^{2}\right) \ln(\nu e^{\gamma_{E}}r)$$

$$+ \left(12a_{1}\beta_{0}^{2} + 10\beta_{0}\beta_{1}\right) \ln^{2}(\nu e^{\gamma_{E}}r) + 8\beta_{0}^{3} \ln^{3}(\nu e^{\gamma_{E}}r) .$$

$$(47)$$

Explicit expression for  $a_i$  can be found in the literature [1, 2, 22, 24, 25, 29, 30]. For ease of reference we display them in the Appendix.

We choose to write the initial matching conditions of the potentials, like Eq. (46), in terms of the (single) factorization scale of the effective theory  $\nu$  and not  $\nu_s$ , as  $\nu_s$  does not appear in a matching computation done order by order in  $\alpha$ . The (left-over) factorization scale dependence of the matching coefficient would cancel with the scale dependence of loops in the effective theory (in practice most of the scale dependence in the potentials, for instance in Eq. (46), cancels with the scale dependence of  $\alpha(\nu)$ , effectively becoming  $\alpha(1/r)$  but this does not change the physical principle). When a RG analysis is done one introduces

 $<sup>^{3}</sup>$  This observation also applies to the RG corrections to the potentials obtained in the previous subsection.

two factorization scales: the one where the running starts, which we have named  $\nu_s$  in the previous section, and the factorization scale that would cancel with the scale dependence of loops in the effective theory, which we have always named  $\nu$ . Therefore, the total RG improved static potential then reads

$$V_{s\overline{\text{MS}}}^{(0),RG}(r;\nu) = V_{s\overline{\text{MS}}}^{(0)}(r;\nu_s) + \delta V_{s,RG}^{(0)}(r;\nu_s,\nu),$$
(48)

and it is correct with NNNLL accuracy.

For the 1/m potential the initial matching condition reads

$$V_{s,\overline{\text{MS}}}^{(1)}(r,\nu) = \frac{C_f \alpha^2(\nu)}{2r^2} \left( b_1 + \frac{\alpha(\nu)}{\pi} \left[ b_2 + \left( \frac{b_1 \beta_0}{2} - \frac{2}{3} (C_A^2 + 2C_A C_f) \right) \ln(\nu^2 r^2 e^{2\gamma_E}) \right] \right), \quad (49)$$

where

$$b_1 = \frac{C_f}{2} - C_A, \qquad b_2 = -\frac{89}{36}C_A^2 + \frac{17}{18}C_AC_f + \frac{49}{36}C_AT_Fn_f - \frac{2}{9}C_fT_Fn_f. \tag{50}$$

The two loop result has been taken from Ref. [31] and changed accordingly to fit our renormalization scheme for the ultrasoft computation. This explains the different coefficient  $b_2$  we have compared with that reference. Ours is the proper one to be combined with the ultrasoft correction obtained in Eq. (72) in the next section. The total RG improved 1/m potential then reads

$$V_{s,\overline{\text{MS}}}^{(1),RG}(r;\nu) = V_{s,\overline{\text{MS}}}^{(1)}(r;\nu_s) + \delta V_{s,RG}^{(1)}(r;\nu_s,\nu),$$
(51)

and it is correct with NNLL accuracy.

For the momentum-dependent  $1/m^2$  potential the matching coefficient reads at one loop [3]

$$V_{p^2,\overline{\text{MS}}}^{(2)}(r,\nu) = \frac{C_f \alpha(\nu)}{4} \left( -4 + \frac{\alpha(\nu)}{\pi} \left( -\frac{31}{9} C_A + \frac{20}{9} T_F n_f - \left( \beta_0 + \frac{8}{3} C_A \right) \ln(\nu^2 r^2 e^{2\gamma_E}) \right) \right). \tag{52}$$

The total RG improved momentum-dependent  $1/m^2$  potential then reads

$$V_{p^2,\overline{\rm MS}}^{(2),RG}(r;\nu) = V_{p^2,\overline{\rm MS}}^{(2)}(r;\nu_s) + \delta V_{p^2,RG}^{(2)}(r;\nu_s,\nu), \qquad (53)$$

and it is correct with NLL accuracy.

The results obtained for the above potentials are exact to the required accuracy, since their soft running is trivial and there are not potential loops at this order. This can be traced back to the fact that there is no dependence on the matching coefficients inherited from NRQCD, and no logarithms proportional to the mass appear. The independence of the potential on  $\nu_s$ ,  $\nu_s \frac{dV}{d\nu_s} = 0$ , can be easily implemented by setting  $\nu_s = 1/r$ , giving information on the  $\ln r$  dependence. In fixed-order bound state computations is convenient to work using  $\alpha(\nu_s)$  as the expansion parameter with  $\nu_s \sim m\alpha$ . By expanding  $\alpha(1/r)$  in powers of  $\alpha(\nu_s)$  times  $\ln(\nu_s r)$  subleading corrections appear that have to included with the appropriated precision.

The case of  $V_r^{(2)}$  is different. It depends on the mass of the heavy quark (i.e. on the matching coefficients inherited from NRQCD). In this case we can not give the complete expression with NLL accuracy. For such accuracy we would need the soft divergences to a higher order and the inclusion of effects due to potential divergences. The latter are absorbed in delta-type potentials. Note that when computing their running at NLL the ultrasoft LL running would enter indirectly. Such kind of computations have already been undertaken in Refs. [5, 6] for the spin-dependent corrections to the hyperfine splitting of heavy quarkonium, a similar analysis for the spin-independent corrections would go much beyond the aim of this work. Either way we can still give the NLO matching coefficient for the potential, the relevant starting point for a complete NLL. It is first convenient to write it in terms of the potential in momentum space

$$V_{r,\overline{\text{MS}}}^{(2)}(r,\nu) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \tilde{V}_{r,\overline{\text{MS}}}^{(2)}(q,\nu), \qquad (54)$$

where

$$\tilde{V}_{r,\overline{\text{MS}}}^{(2)}(q,\nu) = \pi C_f \left[ \alpha(q) (1 + c_D(\nu) - 2c_F^2(\nu)) + \frac{1}{\pi} (d_{vs}(\nu) + 3d_{vv}(\nu) + \frac{1}{C_f} (d_{ss}(\nu) + 3d_{vv}(\nu))) + \delta \tilde{V}_{soft}(\nu,q) \right],$$
(55)

$$\delta \tilde{V}_{soft} = \frac{\alpha^2}{\pi} \left[ \left( \frac{9}{4} + \frac{25}{6} \ln \frac{\nu^2}{q^2} \right) C_A + \left( \frac{1}{3} - \frac{7}{3} \ln \frac{\nu^2}{q^2} \right) C_f \right]. \tag{56}$$

The soft one-loop result  $\delta \tilde{V}_{soft}$  is taken from Ref. [3]. The rest corresponds to the hard contribution. We have checked that upon expanding the NRQCD matching coefficients in powers of  $\alpha(\nu_s)$  we agree with that reference at  $\mathcal{O}(\alpha^2)$ . In order to use  $\delta \tilde{V}_{soft}$  we had to change the scheme used for the Pauli  $\sigma$  matrices in the computation of  $d_{vv}$  in Ref. [32] (see also the discussion in Refs. [13, 33]). The new expression for  $d_{vv}$  can be found in the

Appendix, as well as for the other NRQCD matching coefficients. Eq. (54) is correct at LO, LL (soft). It is also correct at NLO, providing with the right initial matching condition to compute the NLL result. We can then give the following expression for the potential

$$V_{r,\overline{\text{MS}}}^{(2),RG}(r;\nu) = V_{r,\overline{\text{MS}}}^{(2)}(r;\nu_s) + \delta V_{r,RG}^{(2)}(r;\nu_s,\nu).$$
 (57)

This expression does not incorporate the NLL running associated to the Fourier transform of  $\ln q$  yet. In order to do so it is rather more convenient to consider

$$V_{r,\overline{\text{MS}}}^{(2),RG}(r;\nu) = V_{r,\overline{\text{MS}}}^{(2)}(r) + \delta V_{r,RG}^{(2)}(r;\nu), \qquad (58)$$

where

$$V_{r,\overline{\text{MS}}}^{(2)}(r) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \tilde{V}_{r,\overline{\text{MS}}}^{(2)}(q,q).$$
 (59)

Although this new expression, Eq. (58), does not account for all the logs at NLL order, yet it does for the ultrasoft logs and those associated to  $\ln q$ . This is enough for the computation of the mass of the  $l \neq 0$  and s = 0 states with NNNLL accuracy. The reason is that the delta potential does not contribute to the mass of those states. This is more clearly seen if we Taylor expand the above expression in powers of (the Fourier transform of)  $\ln q$ :

$$V_{r,\overline{\text{MS}}}^{(2),RG}(r;\nu) = \delta^{3}(\mathbf{r}) \left( \tilde{V}_{r,\overline{\text{MS}}}^{(2)}(\nu_{s},\nu_{s}) + \delta \tilde{V}_{r,RG}^{(2)}(\nu_{s};\nu_{s},\nu) \right) - (\ln \nu_{s}) q \frac{d}{dq} (\tilde{V}_{r,\overline{\text{MS}}}^{(2)}(q,q) + \delta \tilde{V}_{r,RG}^{(2)}(q;q,\nu))|_{q=\nu_{s}} \right) - \frac{1}{4\pi} \left( \text{reg} \frac{1}{r^{3}} \right) q \frac{d}{dq} (\tilde{V}_{r,\overline{\text{MS}}}^{(2)}(q,q) + \delta \tilde{V}_{r,RG}^{(2)}(q;q,\nu))|_{q=\nu_{s}} + \cdots,$$
 (60)

where we have used

$$-\frac{1}{4\pi} \left( \operatorname{reg} \frac{1}{r^3} \right) \equiv \int \frac{d^3 q}{(2\pi)^3} e^{i\mathbf{q} \cdot \mathbf{r}} \ln q \,. \tag{61}$$

Only the term proportional to  $\operatorname{reg} \frac{1}{r^3}$  contributes to the mass of the states with  $l \neq 0$ . Higher order terms in the Taylor expansion are subleading. The derivative of the potential can be basically written in terms of the NRQCD matching coefficients

$$q\frac{d}{dq}\tilde{V}_{r,\overline{MS}}^{(2)}(q,q)|_{q=\nu_s} = C_f \alpha^2(\nu_s) \left[ \frac{2}{3} T_F n_f (c_D + c_1^{hl}) + (\beta_0 - \frac{13}{3} C_A) c_F^2 - \frac{\beta_0}{2} + (\frac{14}{3} C_f - \frac{2}{3} C_A) c_k^2 \right],$$
(62)

$$q\frac{d}{dq}(\delta \tilde{V}_{r,RG}^{(2)}(q;q,\nu))|_{q=\nu_s} = -C_f \alpha^2(\nu_s) \frac{16}{3} \left(\frac{C_A}{2} - C_f\right) \left[1 + \ln \frac{\alpha(\nu_s)}{\alpha(\nu)}\right]. \tag{63}$$

In order to obtain Eq. (60), we have used the explicit  $\alpha(r^{-1})$  dependence of the potential. At the end we have a double expansion in  $\alpha(\nu_s)$  and  $\alpha(\nu)$ . In the bound state calculation they get replaced by  $\nu_s \sim m\alpha$  and  $\nu \sim m\alpha^2$ .

We take Eq. (58) or Eq. (60) as our final expressions for  $V_{r,\overline{\rm MS}}^{(2),RG}(r;\nu)$ .

We have then obtained the RG improved and initial matching coefficients for the different potentials that compose  $V_s$  to the order of interest. As we have already mentioned the 1/m and  $1/m^2$  potentials suffer from field redefinitions ambiguities. Therefore, in some circumstances it can be convenient to cast the initial matching conditions of  $V_s$  in the following unified form<sup>4</sup>:

$$V_{s,\overline{\text{MS}}}(r;\nu_s) = V_{s,\overline{\text{MS}}}^{(0)}(r;\nu_s) + \frac{V_{s,\overline{\text{MS}}}^{(1)}(r;\nu_s)}{m} + \frac{1}{m^2} \left( \frac{1}{2} \left\{ \mathbf{p}^2, V_{\mathbf{p}^2,\overline{\text{MS}}}^{(2)}(r;\nu_s) \right\} + V_{r,\overline{\text{MS}}}^{(2)}(r) \right) , \quad (64)$$

as well as the total potential to be introduced in the Schroedinger equation

$$V_{s,\overline{\text{MS}}}^{RG}(r;\nu) = V_{s,\overline{\text{MS}}}(r;\nu_s = 1/r) + \delta V_{s,RG}(r;\nu_s = 1/r,\nu)$$

$$= V_{s,\overline{\text{MS}}}^{(0),RG}(r;\nu) + \frac{V_{s,\overline{\text{MS}}}^{(1),RG}(r;\nu)}{m} + \frac{1}{m^2} \left(\frac{1}{2} \left\{ \mathbf{p}^2, V_{\mathbf{p}^2,\overline{\text{MS}}}^{(2),RG}(r;\nu) \right\} + V_{r,\overline{\text{MS}}}^{(2),RG}(r;\nu) \right).$$
(65)

Note that we have worked in a basis where  $V_{L^2}$  is set to zero, at least within the accuracy of our computation.

#### IV. OBSERVABLES

#### A. Static potential and Energy

The singlet static energy can be considered to be an observable for our purposes. It does not suffer from field redefinitions ambiguities and can be easily compared with the lattice determination. It consists of the static potential, which is a Wilson coefficient, and an ultrasoft contribution, both of them can be taken either bare or renormalized. More explicitly, the expression for the static energy with NNNLL precision reads

$$E_s(r) = V_{s,\overline{MS}}^{(0),RG}(r;\nu = \Delta V) + \delta E_{s,\overline{MS}}^{(0),us}(r;\nu = \Delta V),$$
(66)

 $<sup>^4</sup>$  Note that we use  $V_{r,\overline{\rm MS}}^{(2)}(r)$  and not  $V_{r,\overline{\rm MS}}^{(2)}(r,\nu_s).$ 

where

$$\delta E_{s,\overline{\text{MS}}}^{(0),us}(r,\nu) = -C_f \mathbf{r}^2 (\Delta V)^3 V_A^2 \frac{\alpha(\nu)}{9\pi} \left( 6 \ln \frac{\Delta V}{\nu} + 6 \ln 2 - 5 \right). \tag{67}$$

Note that one has to be careful in using the same scheme in the soft and ultrasoft to obtain the correct result for the energy of the static singlet state. For ease of reference we also give the NNNLO result. It reads

$$E_s^{NNNLO}(r) = V_{s,\overline{\text{MS}}}^{(0)}(r;\nu) + \delta E_{s,\overline{\text{MS}}}^{(0),us}(r;\nu).$$
 (68)

We can also give the expression for the subleading ultrasoft contribution to the static energy:

$$\delta E_{s,\overline{\text{MS}}}^{(0),us}|_{\text{NLO}} = C_f \mathbf{r}^2 (\Delta V)^3 V_A^2 \frac{\alpha^2(\nu)}{108\pi^2} \left( 18\beta_0 \ln^2 \left( \frac{\Delta V}{\nu} \right) \right) 
-6 \left( C_A \left( 13 + 4\pi^2 \right) - 2\beta_0 (-5 + 3\ln 2) \right) \ln \left( \frac{\Delta V}{\nu} \right) 
-2C_A \left( -84 + 39\ln 2 + 4\pi^2 (-2 + 3\ln 2) + 72\zeta(3) \right) + \beta_0 \left( 67 + 3\pi^2 - 60\ln 2 + 18\ln^2 2 \right) \right).$$
(69)

This contribution is relevant for the complete N<sup>4</sup>LO or N<sup>4</sup>LL computation of the static energy. For the former the only computation left is the soft four-loop contribution to the static potential.

#### **B.** Energy $l \neq 0$ s = 0

We are now in the position to obtain the heavy quarkonium energy with N<sup>3</sup>LL accuracy (for  $l \neq 0$  and s = 0):

$$E_{nljs}|_{l\neq 0,s=0} = \left(E_{\overline{\text{MS}},nljs}^{pot} + \delta E_{\overline{\text{MS}},nl}^{us}\right)|_{l\neq 0,s=0},$$

$$(70)$$

where  $E_{\overline{\text{MS}} nlis}^{pot}$  is the eigenvalue of the equation

$$\left(\frac{p^2}{2m_r} + V_{s,\overline{\text{MS}}}^{RG}\right)\phi_{njls}(\mathbf{r}) = E_{\overline{\text{MS}},nljs}^{pot}\phi_{nljs}(\mathbf{r}),$$
(71)

and  $V_{s,\overline{\text{MS}}}^{RG}$  is Eq. (65) minus  $\left(\frac{1}{8m_1^3} + \frac{1}{8m_2^3}\right) \mathbf{p}^4$ .

The exact solution of Eq. (71) correctly produces all necessary soft and potential terms for the aimed N<sup>3</sup>LL accuracy, as well as some subleading terms. Such exact solution would only be possible to obtain through numerical methods (which on the other hand could

actually be more easy to implement in practice). If we want to restrict ourselves to a strict  $N^3LL$  computation (in particular if seeking for an explicit analytical result), Eq. (71) should be computed within quantum mechanics perturbation theory up to NNNLO for general quantum numbers. Up to NNLO such computation was performed in Ref. [34]. The lengthy  $N^3LO$  computation is missing, beyond the aim of this work, and will be considered elsewhere (for l = 0 and n = 1 such computation has been performed in Ref. [4]).

The ultrasoft correction to the energy due to the ultrasoft correction can be written in the following compact form

$$\delta E_{\overline{\text{MS}},nl}^{us} = \langle n, l | \left( C_f \mathbf{r} (h_o - E_{n,l})^3 V_A^2 \left[ -\frac{\alpha}{9\pi} \left( 6 \ln \left( \frac{h_o - E_{n,l}}{\nu} \right) + 6 \ln 2 - 5 \right) \right. \right. \\
\left. + \frac{\alpha^2}{108\pi^2} \left( 18\beta_0 \ln^2 \left( \frac{h_o - E_{n,l}}{\nu} \right) - 6 \left( N_c \left( 13 + 4\pi^2 \right) - 2\beta_0 (-5 + 3 \ln 2) \right) \ln \left( \frac{h_o - E_{n,l}}{\nu} \right) \right. \\
\left. + 2C_A \left( 84 - 39 \ln 2 + 4\pi^2 (2 - 3 \ln 2) - 72\zeta(3) \right) + \beta_0 \left( 67 + 3\pi^2 - 60 \ln 2 + 18 \ln^2 2 \right) \right) \right] \mathbf{r} \right) |n, l\rangle ,$$

where the states  $|n,l\rangle$  and the energies  $E_{n,l}$  used above are the solution of the Schroedinger potential including the 1-loop static potential (i.e. with NLO accuracy):

$$\left[\frac{\mathbf{p}^2}{2m_r} - \frac{C_f \alpha_s(\nu)}{r} \left\{ 1 + \frac{\alpha_s(\nu)}{4\pi} a_1(\nu; r) \right\} \right] |n, l\rangle = E_{n, l} |n, l\rangle.$$
 (73)

 $h_o$  could also be approximated to its NLO expression:

$$h_o = \frac{\mathbf{p}^2}{2m_r} + \frac{1}{2N_c} \frac{\alpha_s(\nu)}{r} \left\{ 1 + \frac{\alpha_s(\nu)}{4\pi} a_1(\nu; r) \right\}.$$
 (74)

Eq. (72) includes the complete LO  $\mathcal{O}(m\alpha^5)$  and NLO  $\mathcal{O}(m\alpha^6)$  ultrasoft effects, as well as subleading effects. The LO expression would be enough for the N<sup>3</sup>LL precision. A semianalytic expression exists for l=0 states [25] but missing for general quantum numbers and would require a dedicated study, again beyond the aim of this paper. In a strict fixed-order computation one should expand the wave functions to the appropriate order, as well as  $h_o - E_{n,l}$ , but in some situations it could be more convenient to handle this expression numerically.

## V. CONCLUSIONS

We have computed the NLL ultrasoft running of the spin-independent singlet potentials up to  $\mathcal{O}(1/m^2)$ , and the corresponding contribution to the spectrum. This includes the static energy at NNNLL order.

Whereas there are still some pieces left for a complete NNNLL evaluation of the heavy quarkonium spectrum, our result provides with the missing link for the complete result for  $l \neq 0$  and s = 0 states, the structure of which is given in this paper for the first time. The full explicit analytic form will be presented elsewhere.

Another by-product of our computation is the N<sup>4</sup>LO ultrasoft spin-independent contribution to the heavy quarkonium mass and static energy.

Note added: After our paper appeared on the web, the preprint [35] was sent to the arXives. In this reference expressions for the NLL ultrasoft running of the 1/m and  $1/m^2$  potentials were given in the vNRQCD framework and agreement with our results claimed. Note that in order the expressions for the  $1/m^2$  potentials to be equal, the contribution associated to Eq. 31 in [35] has to be added to the result obtained in Ref. [14]. It also remains to be explained how (and if) the dependence on the infrared regulator mentioned in Ref. [18] has disappeared.

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## Appendix A: Constants

$$T_F = \frac{1}{2}; \quad C_A = N_c; \quad C_f = \frac{N_c^2 - 1}{2N_c}.$$
 (A1)

$$\beta_0 = 11 \frac{C_A}{3} - \frac{4}{3} T_F n_f; \qquad \beta_1 = 34 \frac{C_A^2}{3} - \frac{20}{3} C_A T_F n_f - 4 C_f T_F n_f;$$
 (A2)

$$\beta_2 = \frac{2857}{54} C_A^3 - \frac{1415}{27} C_A^2 T_F n_f + \frac{158}{27} C_A T_F^2 n_f^2 - \frac{205}{9} C_A C_f T_F n_f + \frac{44}{9} C_f T_F^2 n_f^2 + 2C_f^2 T_F n_f.$$
 (A3)

$$a_1 = \frac{31C_A - 20T_F n_f}{9};\tag{A4}$$

$$a_{2} = \frac{400 n_{f}^{2} T_{F}^{2}}{81} - C_{f} n_{f} T_{F} \left(\frac{55}{3} - 16 \zeta(3)\right) + C_{A}^{2} \left(\frac{4343}{162} + \frac{16 \pi^{2} - \pi^{4}}{4} + \frac{22 \zeta(3)}{3}\right) - C_{A} n_{f} T_{F} \left(\frac{1798}{81} + \frac{56 \zeta(3)}{3}\right);$$

$$a_3 = a_3^{(3)} n_f^3 + a_3^{(2)} n_f^2 + a_3^{(1)} n_f + a_3^{(0)}, (A5)$$

where

$$a_{3}^{(3)} = -\left(\frac{20}{9}\right)^{3} T_{F}^{3},$$

$$a_{3}^{(2)} = \left(\frac{12541}{243} + \frac{368\zeta(3)}{3} + \frac{64\pi^{4}}{135}\right) C_{A} T_{F}^{2} + \left(\frac{14002}{81} - \frac{416\zeta(3)}{3}\right) C_{f} T_{F}^{2},$$

$$a_{3}^{(1)} = (-709.717) C_{A}^{2} T_{F} + \left(-\frac{71281}{162} + 264\zeta(3) + 80\zeta(5)\right) C_{A} C_{f} T_{F}$$

$$+ \left(\frac{286}{9} + \frac{296\zeta(3)}{3} - 160\zeta(5)\right) C_{f}^{2} T_{F} + (-56.83(1)) \frac{d_{F}^{abcd} d_{F}^{abcd}}{N_{A}},$$

$$a_{3}^{(0)} = 502.24(1) C_{A}^{3} - 136.39(12) \frac{d_{F}^{abcd} d_{A}^{abcd}}{N_{A}},$$
(A6)

and

$$\frac{d_F^{abcd}d_A^{abcd}}{N_A} = \frac{N_c(N_c^2 + 6)}{48} \,. \tag{A7}$$

The NRQCD matching coefficients have been computed over the years. In Ref. [36] one can find the NRQCD matching coefficients of the one heavy quark sector at NLO, whereas in Ref. [32] one can find them for the two heavy quark sector (although with a difference of scheme for  $d_{vv}$ ). In Ref. [37] the LL soft running of the one heavy quark sector was obtained and in Ref. [38] the LL soft running for the two heavy quark sector.  $\alpha(m)$  has  $n_f$  active light flavours:

$$d_2(m) = \frac{\alpha(m)}{60\pi} T_F,\tag{A8}$$

$$c_F(m) = 1 + \frac{\alpha(m)}{2\pi} (C_f + C_A),$$
 (A9)

$$c_D(m) = 1 + \frac{\alpha(m)}{2\pi} C_A - 16d_2(m).$$
 (A10)

$$d_{ss}^{a}(m) = \alpha^{2}(m)C_{f}\left(\frac{C_{A}}{2} - C_{f}\right)(2 - 2\ln 2 + i\pi) , \qquad (A11)$$

$$d_{sv}^a(m) = 0, (A12)$$

$$d_{vs}^{a}(m) = \frac{\alpha^{2}(m)}{2} \left( -\frac{3}{2} C_{A} + 4C_{f} \right) (2 - 2 \ln 2 + i\pi) , \qquad (A13)$$

$$d_{vv}^{a}(m) = -\pi \alpha(m) \left[ 1 + \frac{\alpha(m)}{\pi} \left( T_{R} \left[ \frac{1}{3} n_{f} \left( 2 \ln 2 - \frac{5}{3} - i\pi \right) - \frac{8}{9} \right] + C_{A} \frac{109}{36} - 4C_{f} \right) \right]. \tag{A14}$$

$$\begin{split} d_{ss}(m) &= -\frac{d_{ss}^{*}(m)}{2N_{c}} - \frac{3d_{sv}^{*}(m)}{2N_{c}} - \frac{N_{c}^{2} - 1}{4N_{c}^{2}} d_{vs}^{*}(m) - 3\frac{N_{c}^{2} - 1}{4N_{c}^{2}} d_{vs}^{*}(m) + \frac{2}{3}C_{f}\left(\frac{C_{A}}{2} - C_{f}\right) \alpha^{2}(m), \\ d_{sv}(m) &= -\frac{d_{ss}^{*}(m)}{2N_{c}} + \frac{d_{sv}^{*}(m)}{4N_{c}^{2}} d_{vs}^{*}(m) + \frac{N_{c}^{2} - 1}{4N_{c}^{2}} d_{vv}^{*}(m) + C_{f}\left(\frac{C_{A}}{2} - C_{f}\right) \alpha^{2}(m), \\ d_{vs}(m) &= -d_{ss}^{*}(m) + 3d_{sv}^{*}(m) + \frac{d_{vs}^{*}(m)}{2N_{c}} + \frac{3d_{vv}^{*}(m)}{2N_{c}} + \alpha^{2}(m)(2C_{f} - \frac{C_{A}}{2}). \end{split}$$
(A15)
$$d_{vv}(m) &= -d_{ss}^{*}(m) + d_{sv}^{*}(m) + \frac{d_{vs}^{*}(m)}{2N_{c}} - \frac{d_{vv}^{*}(m)}{2N_{c}} + \alpha^{2}(m)(2C_{f} - \frac{C_{A}}{2}). \tag{A15}$$

$$We now define &z &= \left[\frac{\alpha(\nu_{s})}{\alpha(m)}\right]^{\frac{1}{2}} \simeq 1 - 1/(2\pi)\alpha(\nu_{s}) \ln(\frac{\nu_{s}}{m}), \\ c_{F}(\nu_{s}) &= c_{F}(m) - 1 + z^{-C_{A}}, \\ c_{D}(\nu_{s}) &= c_{D}(m) - 1 + \frac{9C_{A}}{9C_{A} + 8T_{F}n_{f}} \left\{ -\frac{5C_{A} + 4T_{F}n_{f}}{4C_{A} + 4T_{F}n_{f}} z^{-2C_{A}} + \frac{C_{A} + 16C_{f} - 8T_{F}n_{f}}{2(C_{A} - 2T_{F}n_{f})} + \frac{-7C_{A}^{2} + 32C_{A}C_{f} - 4C_{A}T_{F}n_{f} + 32C_{f}T_{F}n_{f}}{4(C_{A} + T_{F}n_{f})(2T_{F}n_{f} - C_{A})} \\ &+ \frac{8T_{F}n_{f}}{9C_{A}} \left[ z^{-2C_{A}} + \left(\frac{20}{13} + \frac{32}{13C_{A}}\right) \left[1 - z^{-\frac{13C_{A}}{6}} \right] \right] \right\}, \\ d_{ss}(\nu_{s}) &= d_{ss}(m) + 4C_{f}\left(C_{f} - \frac{C_{A}}{2}\right) \frac{\pi}{\beta_{0}} \alpha(m) \left[z^{\beta_{0}} - 1\right], \\ d_{vs}(\nu_{s}) &= d_{vs}(m), \\ d_{vs}(\nu_{s}) &= d_{vs}(m) - (C_{f} - C_{A}) \frac{8\pi}{\beta_{0}} \alpha(m) \left[z^{\beta_{0}} - 1\right] \\ &+ \frac{27C_{A}^{2}}{9C_{A} + 8T_{F}n_{f}} \beta_{0}}{4C_{A}} \alpha(m) \left\{ -\frac{5C_{A} + 4T_{F}n_{f}}{4C_{A} + 4T_{F}n_{f}} \frac{\beta_{0}}{\beta_{0} - 2C_{A}} \left(z^{\beta_{0} - 2C_{A}} - 1\right) \right. \\ &+ \frac{C_{A} + 16C_{f} - 8T_{F}n_{f}}{2(C_{A} - 2T_{F}n_{f})} \left\{ z^{\beta_{0}} - 1\right] \\ &+ \frac{7C_{A}^{2} + 32C_{A}C_{f} - 4C_{A}T_{F}n_{f} + 32C_{f}T_{F}n_{f}}{4(C_{A} + T_{F}n_{f}) - 2C_{A}} \left(z^{\beta_{0} - 2C_{A}} - 1\right) \\ &+ \frac{8T_{F}n_{f}}{9C_{A}} \left[ \frac{\beta_{0}}{\beta_{0} - 2C_{A}} \left(z^{\beta_{0} - 2C_{A}} - 1\right) + \left(\frac{20}{13} + \frac{32}{13C_{A}}\right) \\ &\times \left( \left[z^{\beta_{0}} - 1\right] - \frac{6\beta_{0}}{6\beta_{0} - 13C_{A}} \left[z^{\beta_{0} - 13C_{A}} - 1\right] \right) \right] \right\}, \\ d_{vv}(\nu_{s}) &= d_{vv}(m) +$$

The results displayed above for the NRQCD matching coefficients, c's and d's, are correct with LL and NLO accuracy, but not beyond.

We will also need

$$c_1^{hl}(\nu_s) = \frac{9C_A}{9C_A + 8T_F n_f} \left\{ \frac{5C_A + 4T_F n_f}{4C_A + 4T_F n_f} z^{-2C_A} - \frac{C_A + 16C_f - 8T_F n_f}{2(C_A - 2T_F n_f)} - \frac{-7C_A^2 + 32C_A C_f - 4C_A T_F n_f + 32C_f T_F n_f}{4(C_A + T_F n_f)(2T_F n_f - C_A)} z^{4T_F n_f/3 - 2C_A/3} + z^{-2C_A} + \left(\frac{20}{13} + \frac{32}{13} \frac{C_f}{C_A}\right) \left[1 - z^{\frac{-13C_A}{6}}\right] \right\}.$$
(A17)

This is correct with LL accuracy, which is enough for us.

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